



Sample name: **M04_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-24002**
Filename: **C:\Sirius_T3\Mehtap\20180323_exp33_logP_T3-2\18C-24002_M04_octanol_pH-metric high logP.t3r**

Experiment start time: **3/24/2018 1:34:06 AM**
Analyst: **Dorothy Levorse**
Instrument ID: **T312060**

pH-metric Result

logP (XH +) 0.82 ±0.06 (n=50)
logP (neutral X) 4.04 ±0.02 (n=50)
RMSD 0.362

18C-24002 Points 1 to 24

M04_octanol concentration factor 0.923
Carbonate 0.1572 mM
Acidity error -0.23457 mM

18C-24002 Points 25 to 51

M04_octanol concentration factor 0.920
Carbonate 0.1065 mM
Acidity error -0.29812 mM

18C-24002 Points 52 to 75

M04_octanol concentration factor 0.952
Carbonate 0.1039 mM
Acidity error -0.10230 mM

Warnings and errors

Errors None
Warnings None

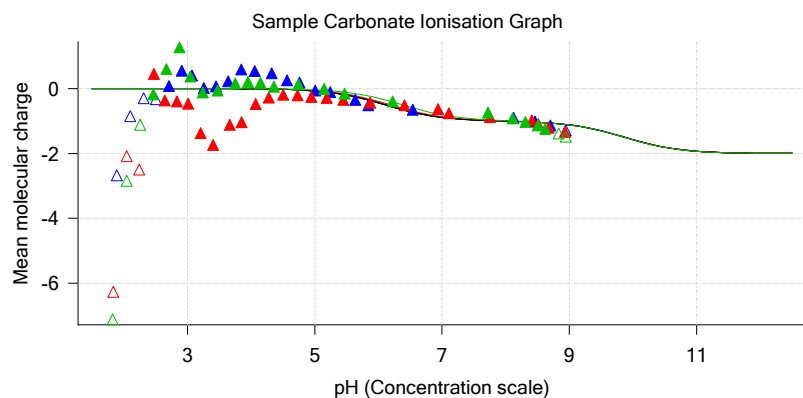
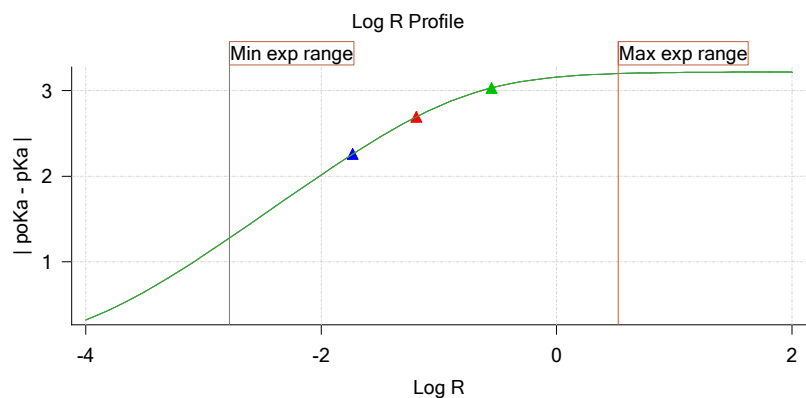
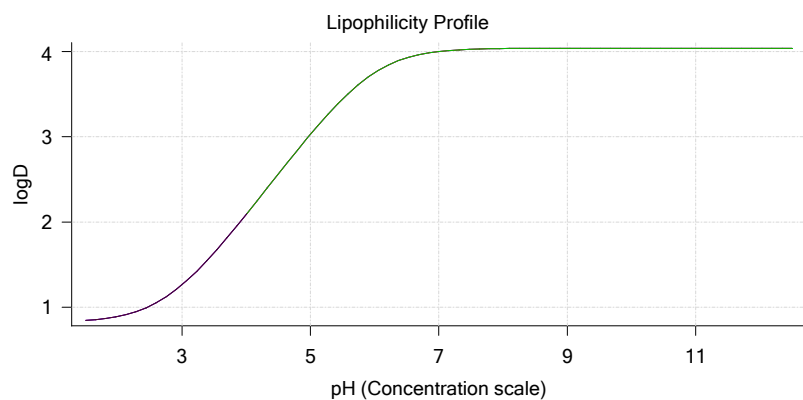
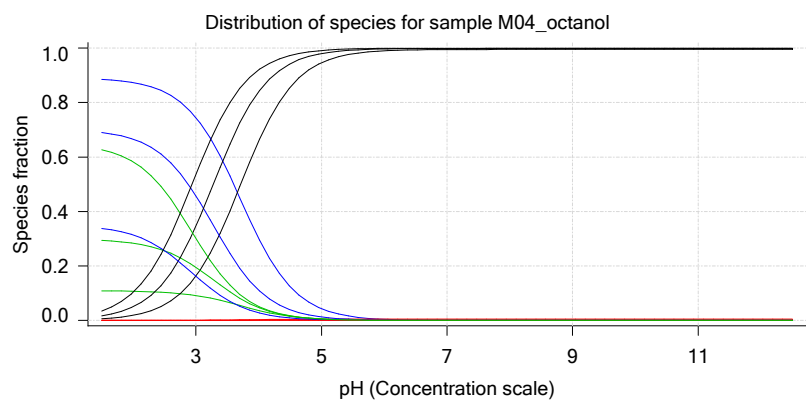
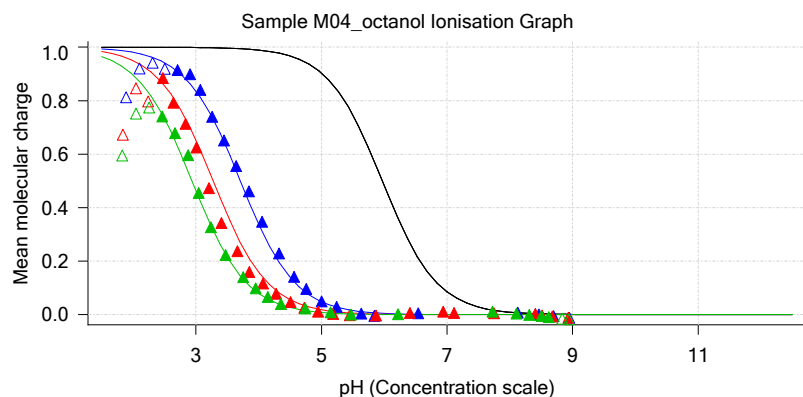
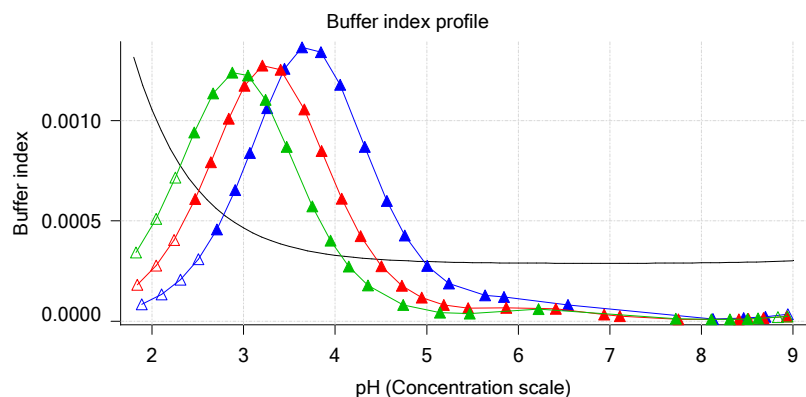
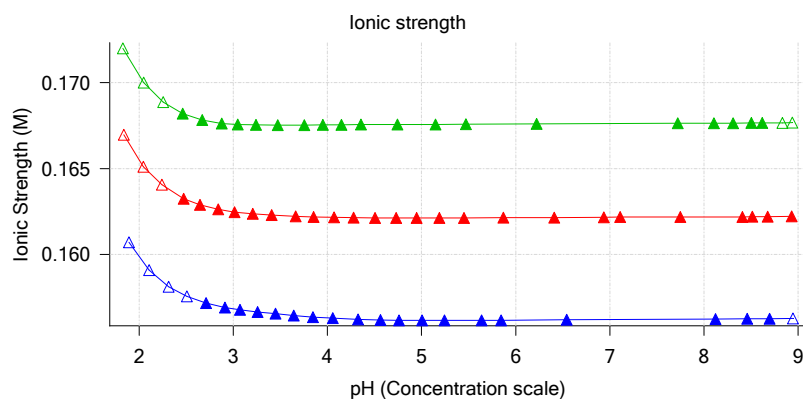
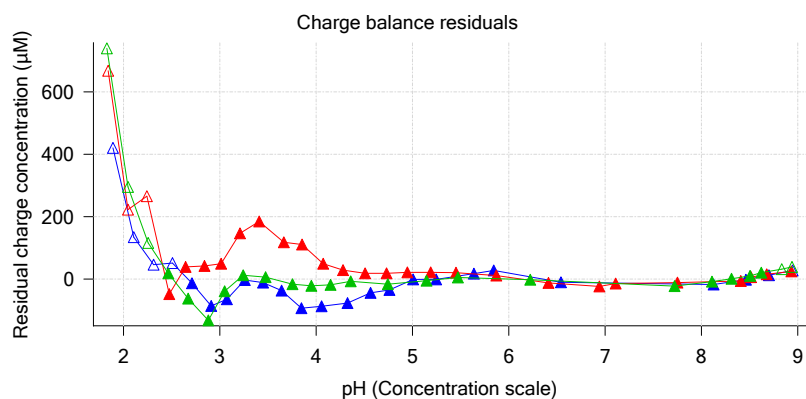
Sample logD and percent species

pH	M04_octanol logD	M04_octanol M04_octanolH	M04_octanol M04_octanol	M04_octanol M04_octanolH*	M04_octanol M04_octanol*	Comment
1.000	0.83	12.93 %	0.00 %	85.56 %	1.52 %	Stomach pH
1.200	0.83	12.81 %	0.00 %	84.80 %	2.38 %	
2.000	0.89	11.37 %	0.00 %	75.28 %	13.34 %	
3.000	1.26	5.17 %	0.01 %	34.21 %	60.62 %	
4.000	2.09	0.80 %	0.01 %	5.30 %	93.89 %	
5.000	3.03	0.08 %	0.01 %	0.56 %	99.35 %	Blood pH
6.000	3.75	0.01 %	0.01 %	0.06 %	99.93 %	
6.500	3.93	0.00 %	0.01 %	0.02 %	99.97 %	
7.000	4.00	0.00 %	0.01 %	0.01 %	99.98 %	
7.400	4.02	0.00 %	0.01 %	0.00 %	99.99 %	
8.000	4.04	0.00 %	0.01 %	0.00 %	99.99 %	
9.000	4.04	0.00 %	0.01 %	0.00 %	99.99 %	
10.000	4.04	0.00 %	0.01 %	0.00 %	99.99 %	
11.000	4.04	0.00 %	0.01 %	0.00 %	99.99 %	
12.000	4.04	0.00 %	0.01 %	0.00 %	99.99 %	

Sample name: **M04_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-24002**
 Filename: **C:\Sirius_T3\Mehtap\20180323_exp33_logP_T3-2\18C-24002_M04_octanol_pH-metric high logP.t3r**

Experiment start time: **3/24/2018 1:34:06 AM**
 Analyst: **Dorothy Levorse**
 Instrument ID: **T312060**

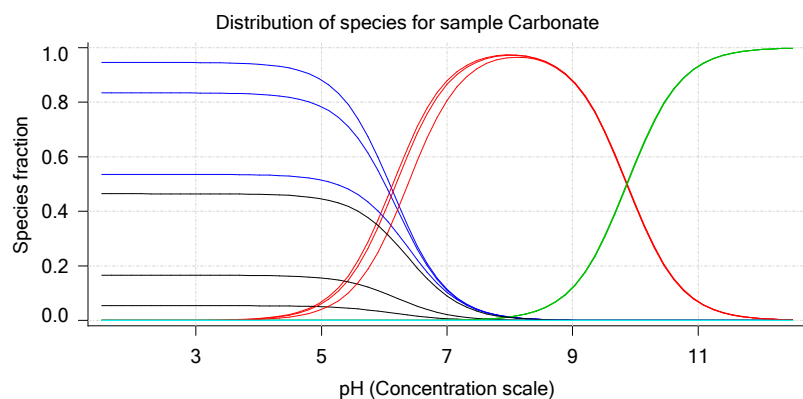
Graphs



Sample name: **M04_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-24002**
 Filename: **C:\Sirius_T3\Mehtap\20180323_exp33_logP_T3-2\18C-24002_M04_octanol_pH-metric high logP.t3r**

Experiment start time: **3/24/2018 1:34:06 AM**
 Analyst: **Dorothy Levorse**
 Instrument ID: **T312060**

Graphs (continued)



Sample name: **M04_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-24002**
 Filename: **C:\Sirius_T3\Mehtap\20180323_exp33_logP_T3-2\18C-24002_M04_octanol_pH-metric high logP.t3r**

Experiment start time: **3/24/2018 1:34:06 AM**
 Analyst: **Dorothy Levorse**
 Instrument ID: **T312060**

pH-metric high logP Titration 1 of 3 18C-24002 Points 1 to 24

Overall results

RMSD 0.282
 Average ionic strength 0.156 M
 Average temperature 24.9°C
 Partition ratio 0.0186 : 1
 Analyte concentration range 2528.6 µM to 2603.3 µM
 Total points considered 19 of 24

Warnings and errors

Errors None
 Warnings None

Four-Plus parameters

Parameter	Value	Date/Time	File
Alpha	0.119	3/24/2018 1:34:06 AM	C:\Sirius_T3\HCl18C23.t3r
S	0.9972	3/24/2018 1:34:06 AM	C:\Sirius_T3\HCl18C23.t3r
jH	0.9	3/24/2018 1:34:06 AM	C:\Sirius_T3\HCl18C23.t3r
jOH	-0.3	3/24/2018 1:34:06 AM	C:\Sirius_T3\HCl18C23.t3r

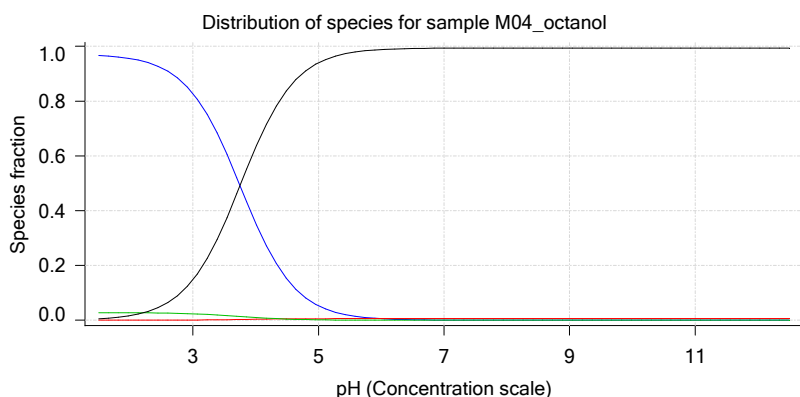
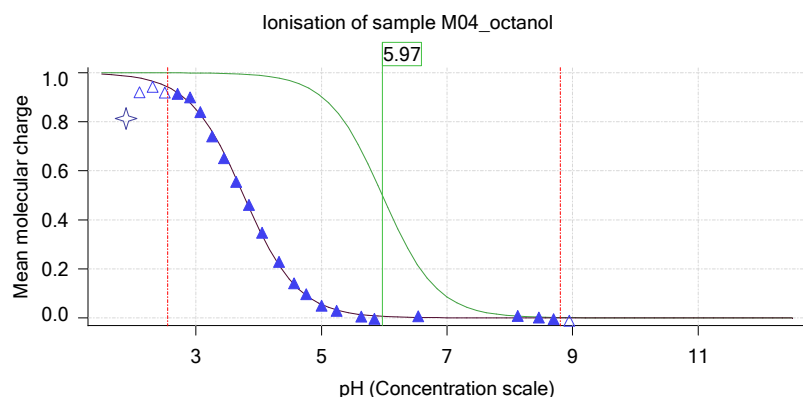
Titrants

Concentration	Value	Date/Time	File
0.50 M HCl	0.997124	3/24/2018 1:34:06 AM	C:\Sirius_T3\HCl18C23.t3r
0.50 M KOH	1.003190	3/24/2018 1:34:06 AM	C:\Sirius_T3\KOH18C23.t3r

Sample

M04_octanol concentration factor	0.923
Base pKa 1	5.97
logP (XH +)	0.19
logP (neutral X)	3.95

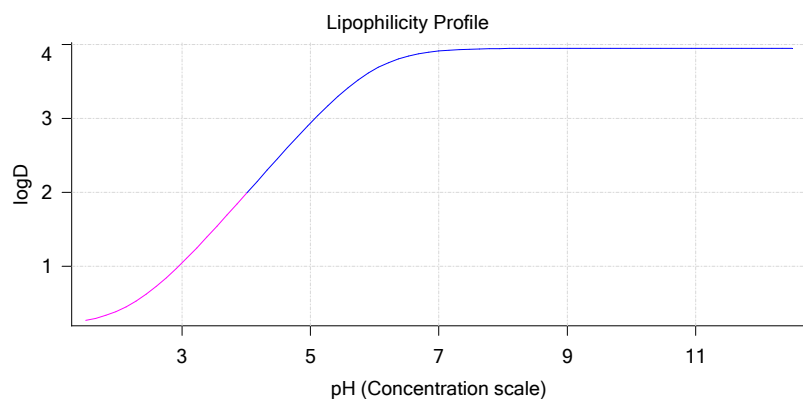
Sample graphs



Sample name: **M04_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-24002**
 Filename: **C:\Sirius_T3\Mehtap\20180323_exp33_logP_T3-2\18C-24002_M04_octanol_pH-metric high logP.t3r**

Experiment start time: **3/24/2018 1:34:06 AM**
 Analyst: **Dorothy Levorse**
 Instrument ID: **T312060**

Sample graphs (continued)



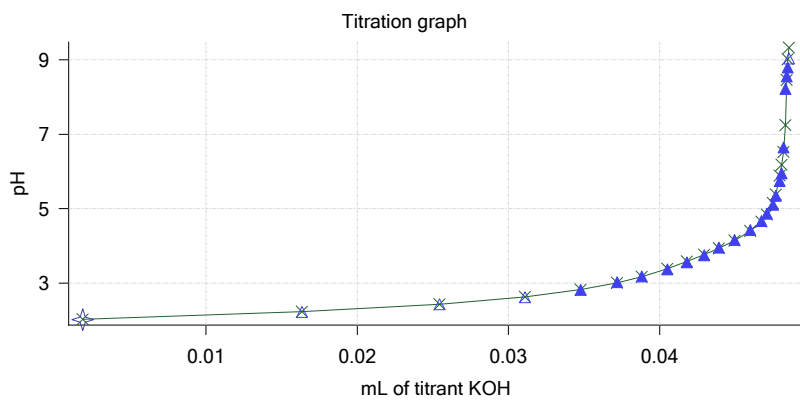
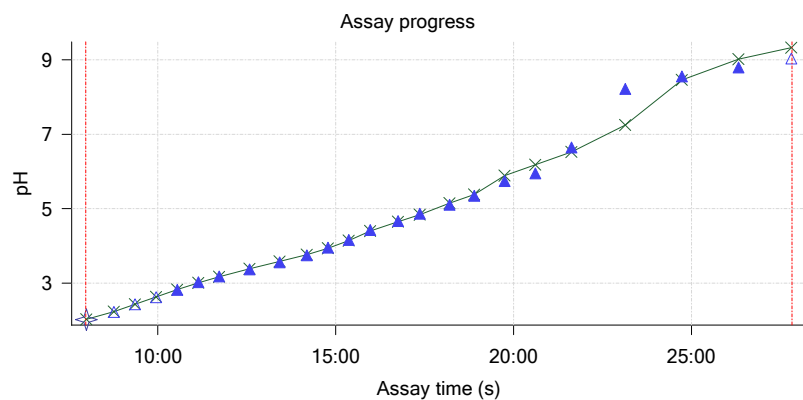
Sample logD and percent species

pH	M04_octanol logD	M04_octanol M04_octanolH	M04_octanol M04_octanol	M04_octanol M04_octanolH*	M04_octanol M04_octanol*	Comment
1.000	0.22	97.04 %	0.00 %	2.79 %	0.17 %	Stomach pH
1.200	0.23	96.94 %	0.00 %	2.79 %	0.27 %	
2.000	0.40	95.55 %	0.01 %	2.75 %	1.70 %	
3.000	1.05	82.83 %	0.09 %	2.38 %	14.70 %	
4.000	1.98	35.54 %	0.38 %	1.02 %	63.06 %	
5.000	2.94	5.30 %	0.57 %	0.15 %	93.98 %	Blood pH
6.000	3.66	0.56 %	0.60 %	0.02 %	98.83 %	
6.500	3.84	0.18 %	0.60 %	0.01 %	99.22 %	
7.000	3.91	0.06 %	0.60 %	0.00 %	99.34 %	
7.400	3.93	0.02 %	0.60 %	0.00 %	99.38 %	
8.000	3.95	0.01 %	0.60 %	0.00 %	99.39 %	
9.000	3.95	0.00 %	0.60 %	0.00 %	99.40 %	
10.000	3.95	0.00 %	0.60 %	0.00 %	99.40 %	
11.000	3.95	0.00 %	0.60 %	0.00 %	99.40 %	
12.000	3.95	0.00 %	0.60 %	0.00 %	99.40 %	

Carbonate and acidity

 Carbonate 0.157 mM
 Acidity error -0.235 mM

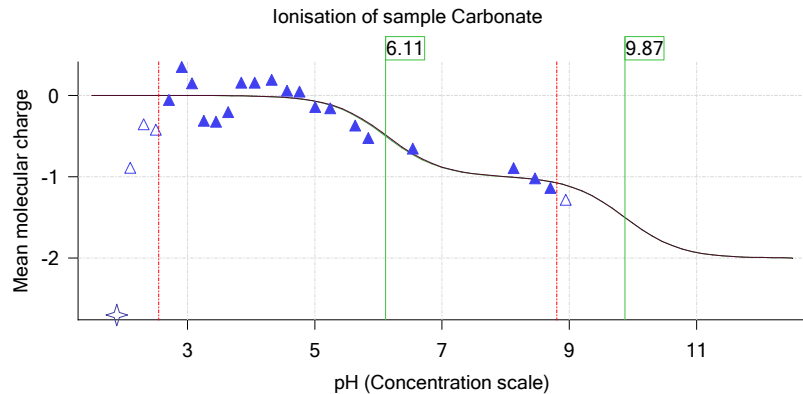
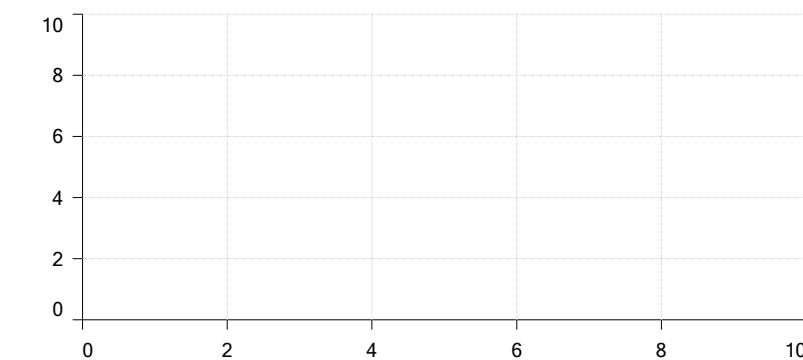
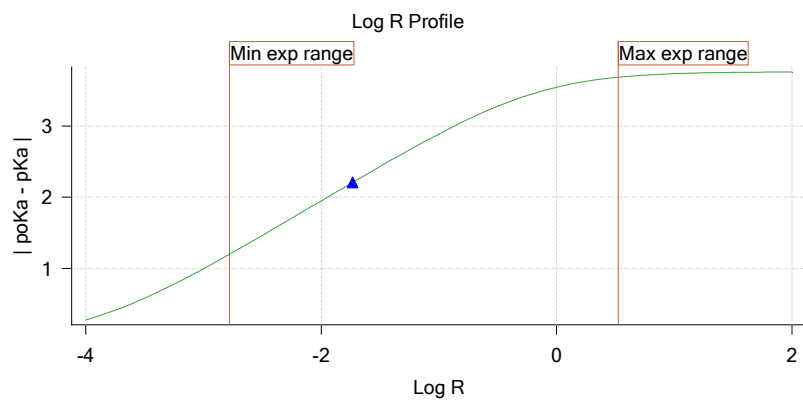
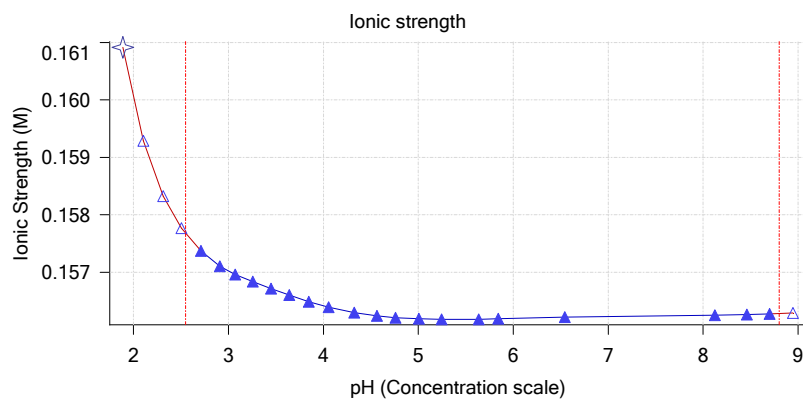
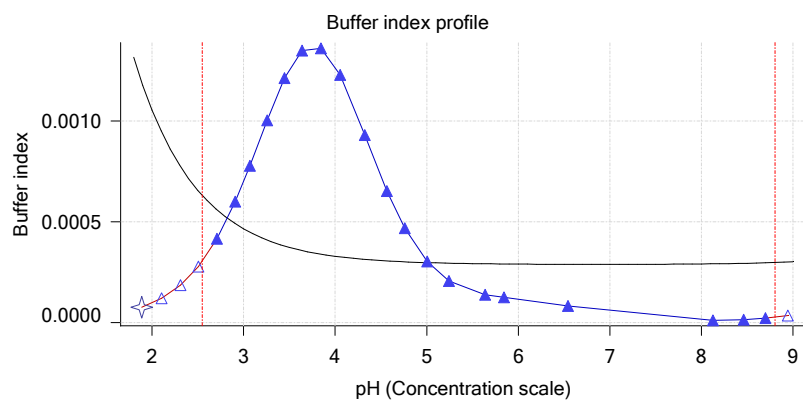
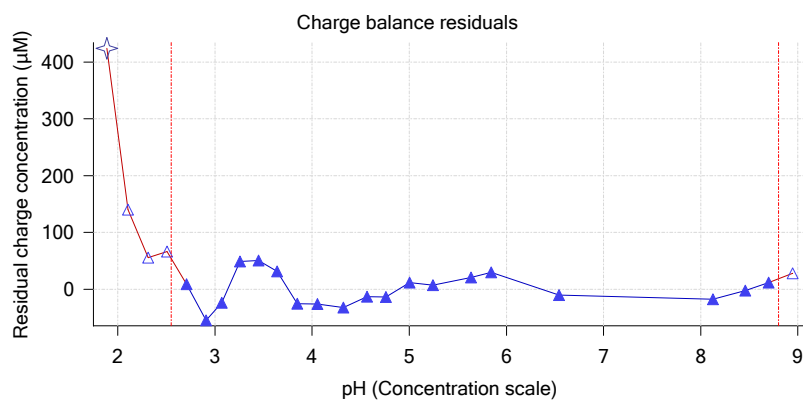
Other graphs



Sample name: **M04_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-24002**
 Filename: **C:\Sirius_T3\Mehtap\20180323_exp33_logP_T3-2\18C-24002_M04_octanol_pH-metric high logP.t3r**

Experiment start time: **3/24/2018 1:34:06 AM**
 Analyst: **Dorothy Levorse**
 Instrument ID: **T312060**

Other graphs (continued)



Sample name: **M04_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-24002**
 Filename: **C:\Sirius_T3\Mehtap\20180323_exp33_logP_T3-2\18C-24002_M04_octanol_pH-metric high logP.t3r**

Experiment start time: **3/24/2018 1:34:06 AM**
 Analyst: **Dorothy Levorse**
 Instrument ID: **T312060**

pH-metric high logP Titration 2 of 3 18C-24002 Points 25 to 51

Overall results

RMSD 0.334
 Average ionic strength 0.162 M
 Average temperature 25.0°C
 Partition ratio 0.0644 : 1
 Analyte concentration range 2267.2 µM to 2336.0 µM
 Total points considered 24 of 27

Warnings and errors

Errors None
 Warnings None

Four-Plus parameters

Alpha 0.119 3/24/2018 1:34:06 AM C:\Sirius_T3\HCl18C23.t3r
 S 0.9972 3/24/2018 1:34:06 AM C:\Sirius_T3\HCl18C23.t3r
 jH 0.9 3/24/2018 1:34:06 AM C:\Sirius_T3\HCl18C23.t3r
 jOH -0.3 3/24/2018 1:34:06 AM C:\Sirius_T3\HCl18C23.t3r

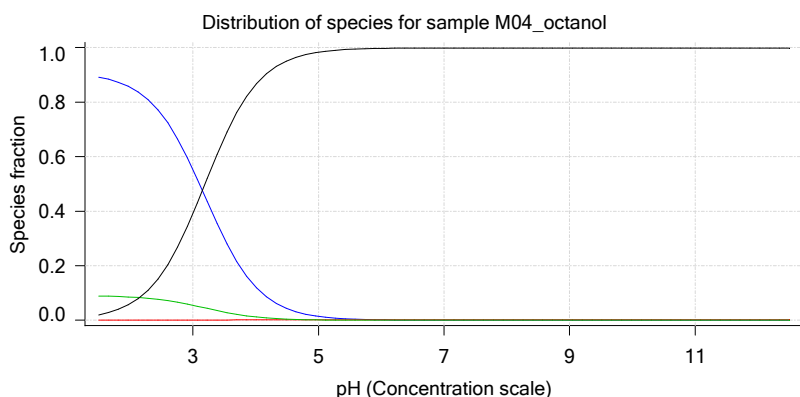
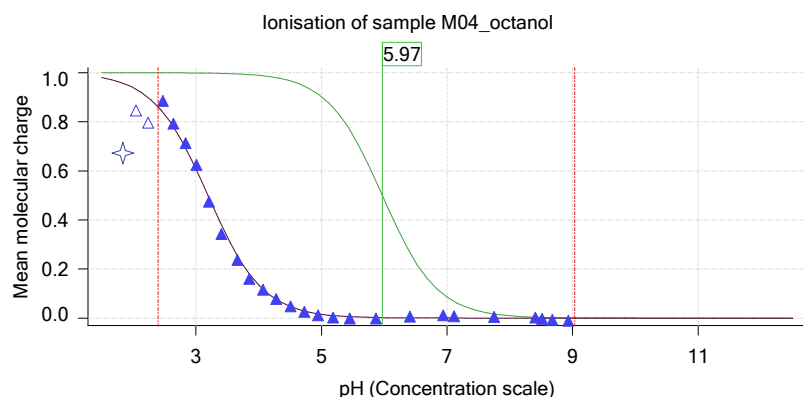
Titrants

0.50 M HCl 0.997124 3/24/2018 1:34:06 AM C:\Sirius_T3\HCl18C23.t3r
 0.50 M KOH 1.003190 3/24/2018 1:34:06 AM C:\Sirius_T3\KOH18C23.t3r

Sample

M04_octanol concentration factor 0.920
 Base pKa 1 5.97
 logP (XH +) 0.19
 logP (neutral X) 4.01

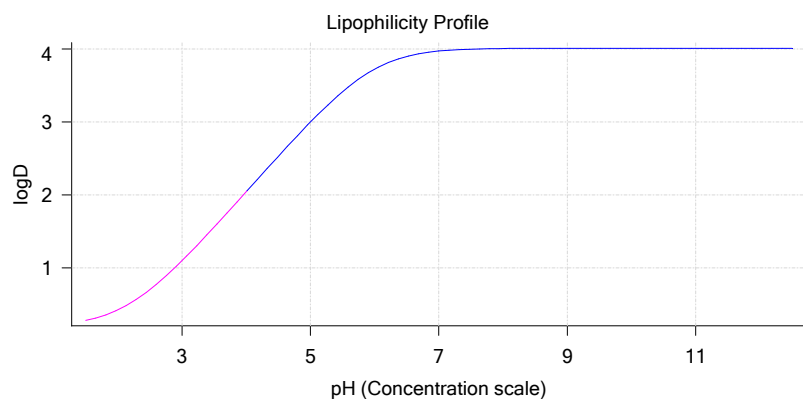
Sample graphs



Sample name: **M04_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-24002**
 Filename: **C:\Sirius_T3\Mehtap\20180323_exp33_logP_T3-2\18C-24002_M04_octanol_pH-metric high logP.t3r**

Experiment start time: **3/24/2018 1:34:06 AM**
 Analyst: **Dorothy Levorse**
 Instrument ID: **T312060**


Sample graphs (continued)



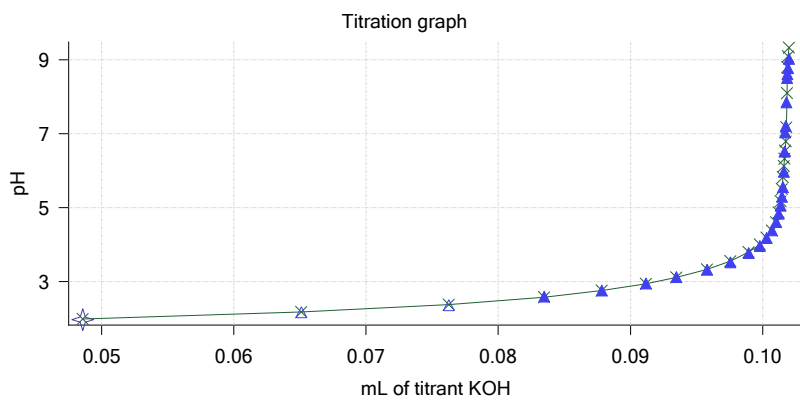
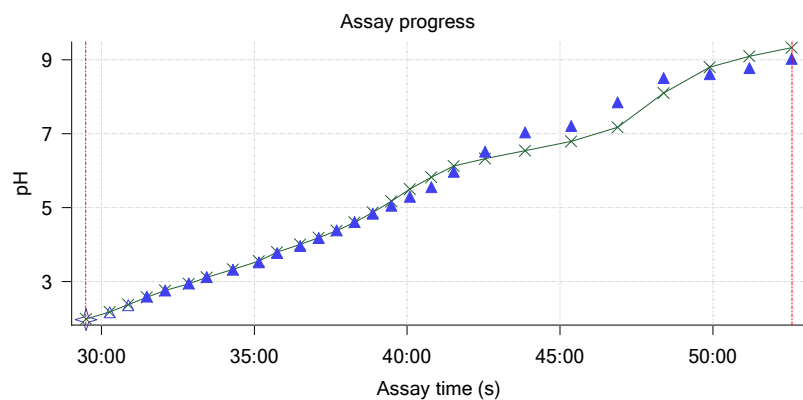
Sample logD and percent species

pH	M04_octanol logD	M04_octanol M04_octanolH	M04_octanol M04_octanol	M04_octanol M04_octanolH*	M04_octanol M04_octanol*	Comment
1.000	0.22	90.35 %	0.00 %	9.01 %	0.64 %	Stomach pH
1.200	0.24	90.02 %	0.00 %	8.97 %	1.01 %	
2.000	0.42	85.44 %	0.01 %	8.52 %	6.03 %	
3.000	1.10	55.36 %	0.06 %	5.52 %	39.07 %	
4.000	2.04	12.24 %	0.13 %	1.22 %	86.40 %	
5.000	3.00	1.39 %	0.15 %	0.14 %	98.32 %	Blood pH
6.000	3.72	0.14 %	0.15 %	0.01 %	99.69 %	
6.500	3.90	0.04 %	0.15 %	0.00 %	99.80 %	
7.000	3.97	0.01 %	0.15 %	0.00 %	99.83 %	
7.400	3.99	0.01 %	0.15 %	0.00 %	99.84 %	
8.000	4.01	0.00 %	0.15 %	0.00 %	99.85 %	
9.000	4.01	0.00 %	0.15 %	0.00 %	99.85 %	
10.000	4.01	0.00 %	0.15 %	0.00 %	99.85 %	
11.000	4.01	0.00 %	0.15 %	0.00 %	99.85 %	
12.000	4.01	0.00 %	0.15 %	0.00 %	99.85 %	

Carbonate and acidity

 Carbonate 0.106 mM
 Acidity error -0.298 mM

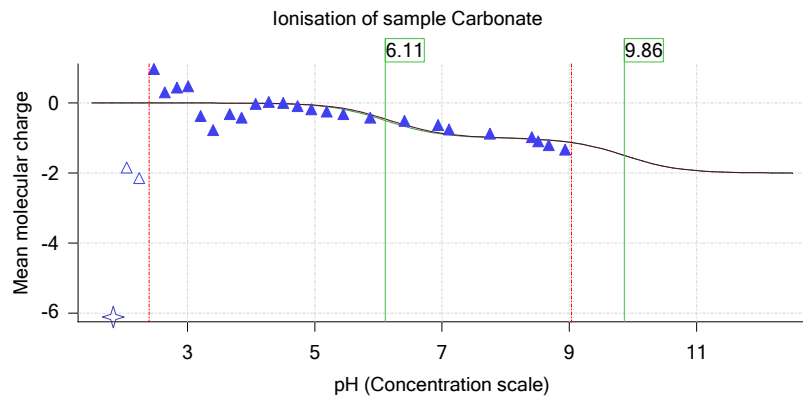
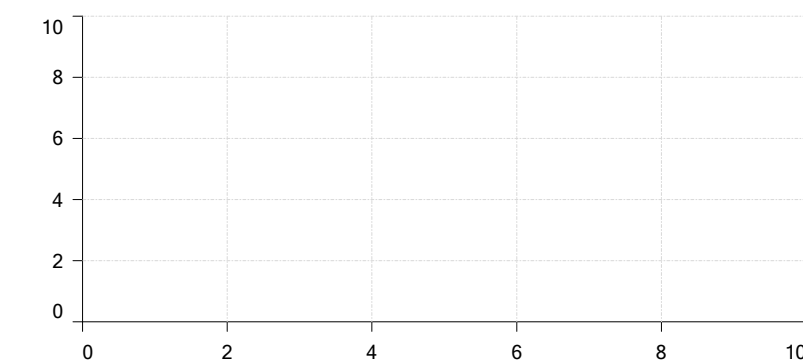
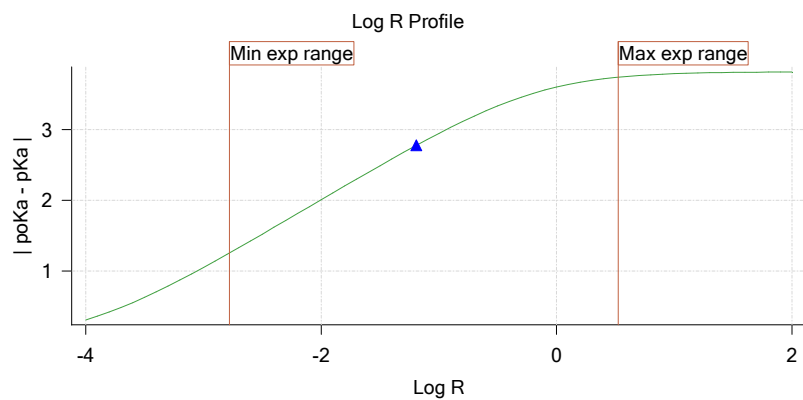
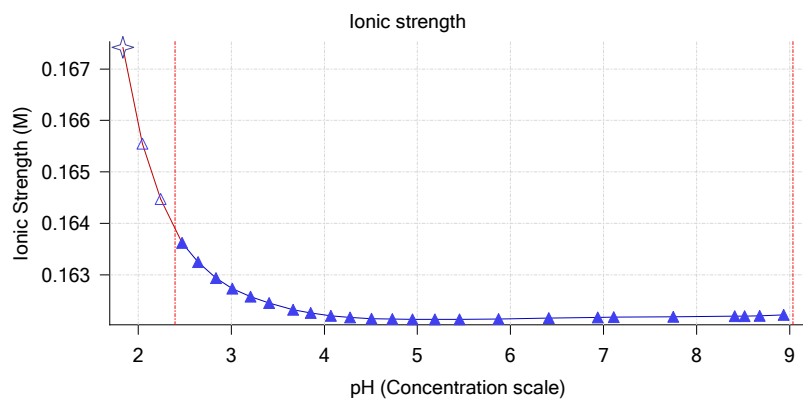
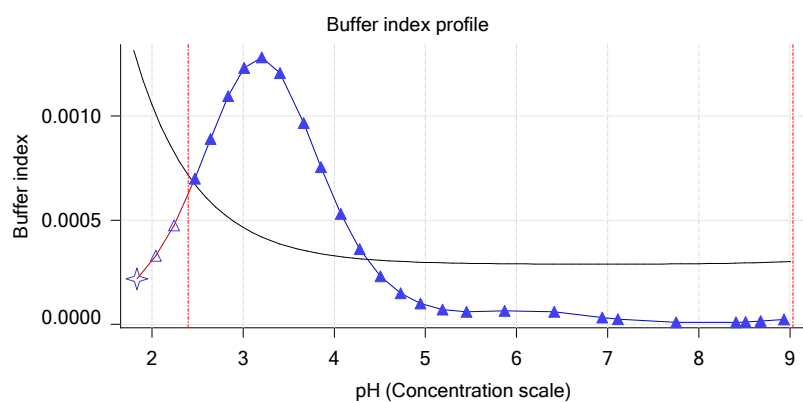
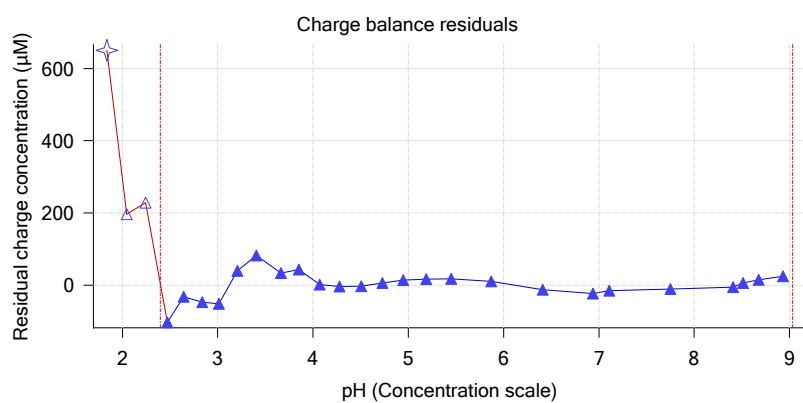
Other graphs



Sample name: **M04_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-24002**
 Filename: **C:\Sirius_T3\Mehtap\20180323_exp33_logP_T3-2\18C-24002_M04_octanol_pH-metric high logP.t3r**

Experiment start time: **3/24/2018 1:34:06 AM**
 Analyst: **Dorothy Levorse**
 Instrument ID: **T312060**

Other graphs (continued)



Sample name: **M04_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-24002**
 Filename: **C:\Sirius_T3\Mehtap\20180323_exp33_logP_T3-2\18C-24002_M04_octanol_pH-metric high logP.t3r**

Experiment start time: **3/24/2018 1:34:06 AM**
 Analyst: **Dorothy Levorse**
 Instrument ID: **T312060**

pH-metric high logP Titration 3 of 3 18C-24002 Points 52 to 75





Overall results

RMSD 0.452
 Average ionic strength 0.168 M
 Average temperature 25.0°C
 Partition ratio 0.2805 : 1
 Analyte concentration range 1766.3 µM to 1811.0 µM
 Total points considered 19 of 24



Warnings and errors

Errors None
 Warnings None





Four-Plus parameters

	Alpha	0.119	3/24/2018 1:34:06 AM	C:\Sirius_T3\HCl18C23.t3r
	S	0.9972	3/24/2018 1:34:06 AM	C:\Sirius_T3\HCl18C23.t3r
	jH	0.9	3/24/2018 1:34:06 AM	C:\Sirius_T3\HCl18C23.t3r
	jOH	-0.3	3/24/2018 1:34:06 AM	C:\Sirius_T3\HCl18C23.t3r

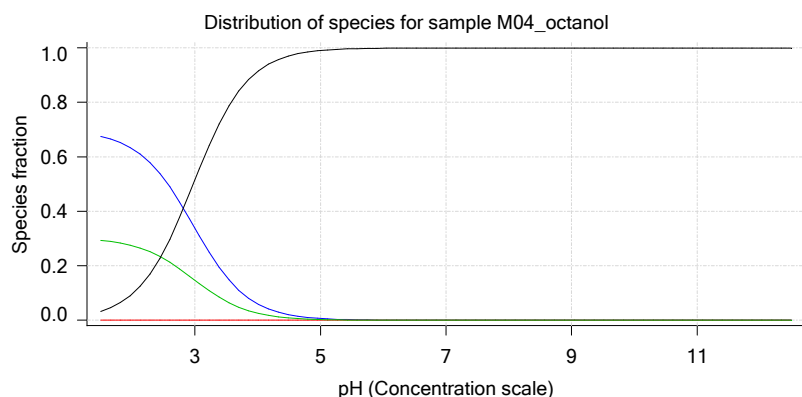
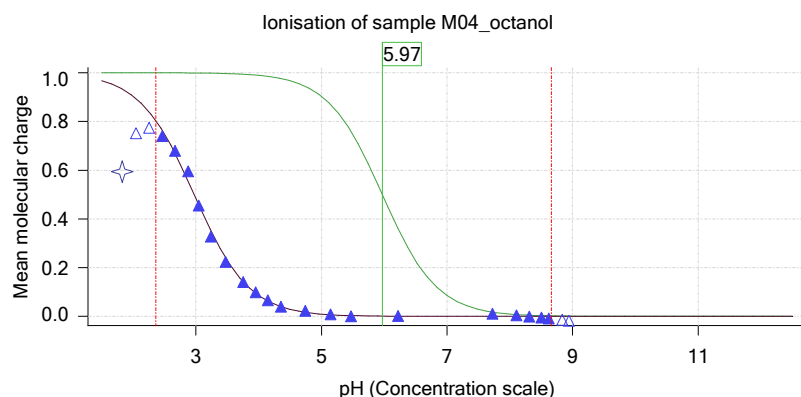
Titrants

	0.50 M HCl	0.997124	3/24/2018 1:34:06 AM	C:\Sirius_T3\HCl18C23.t3r
	0.50 M KOH	1.003190	3/24/2018 1:34:06 AM	C:\Sirius_T3\KOH18C23.t3r

Sample

	M04_octanol concentration factor	0.952
	Base pKa 1	5.97
	logP (XH +)	0.19
	logP (neutral X)	3.70

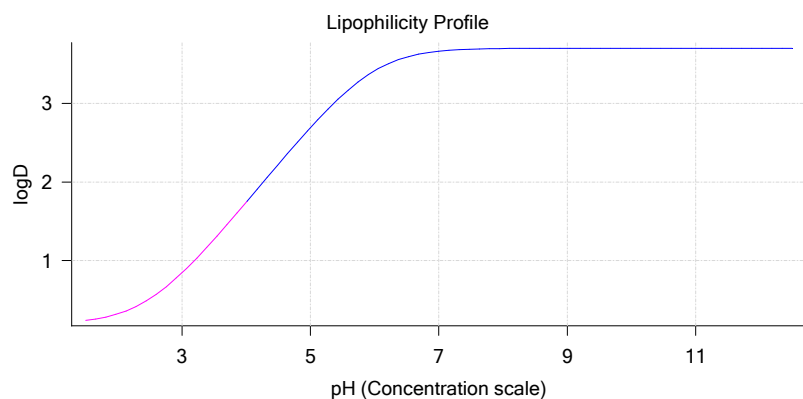
Sample graphs



Sample name: **M04_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-24002**
 Filename: **C:\Sirius_T3\Mehtap\20180323_exp33_logP_T3-2\18C-24002_M04_octanol_pH-metric high logP.t3r**

Experiment start time: **3/24/2018 1:34:06 AM**
 Analyst: **Dorothy Levorse**
 Instrument ID: **T312060**



Sample graphs (continued)



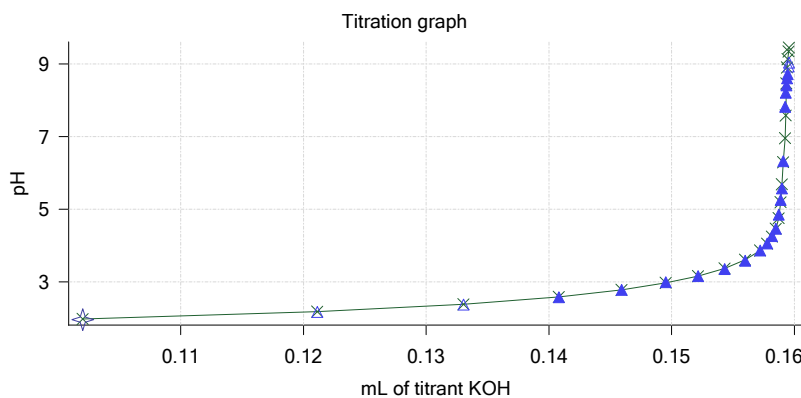
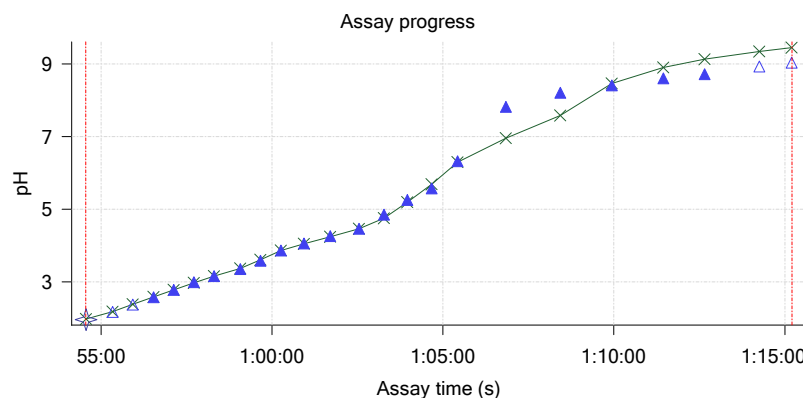
Sample logD and percent species

pH	M04_octanol logD	M04_octanol M04_octanolH	M04_octanol M04_octanolH	M04_octanol M04_octanolH*	M04_octanol M04_octanol*	Comment
1.000	0.20	68.98 %	0.00 %	29.97 %	1.05 %	
1.200	0.21	68.56 %	0.00 %	29.78 %	1.65 %	
2.000	0.32	63.02 %	0.01 %	27.38 %	9.60 %	
3.000	0.84	33.81 %	0.04 %	14.69 %	51.47 %	
4.000	1.74	6.00 %	0.06 %	2.61 %	91.33 %	
5.000	2.69	0.65 %	0.07 %	0.28 %	99.00 %	
6.000	3.42	0.07 %	0.07 %	0.03 %	99.84 %	
6.500	3.59	0.02 %	0.07 %	0.01 %	99.90 %	
7.000	3.67	0.01 %	0.07 %	0.00 %	99.92 %	
7.400	3.69	0.00 %	0.07 %	0.00 %	99.93 %	
8.000	3.70	0.00 %	0.07 %	0.00 %	99.93 %	
9.000	3.70	0.00 %	0.07 %	0.00 %	99.93 %	
10.000	3.70	0.00 %	0.07 %	0.00 %	99.93 %	
11.000	3.70	0.00 %	0.07 %	0.00 %	99.93 %	
12.000	3.70	0.00 %	0.07 %	0.00 %	99.93 %	

Carbonate and acidity

 Carbonate 0.104 mM
 Acidity error -0.102 mM

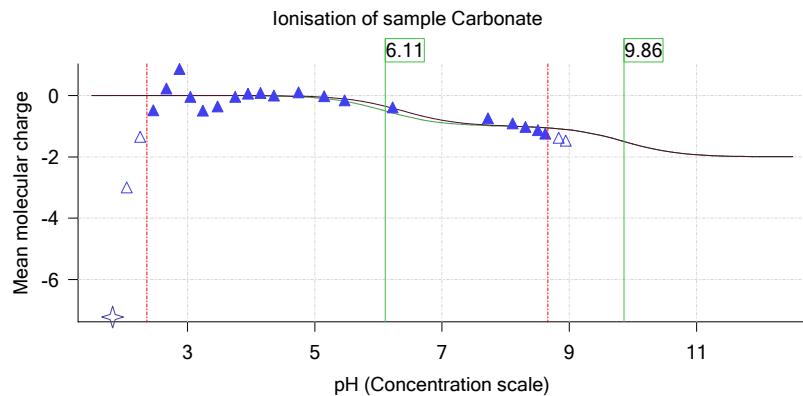
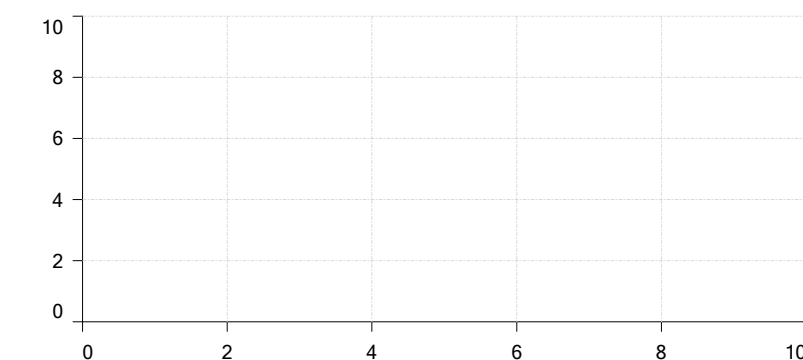
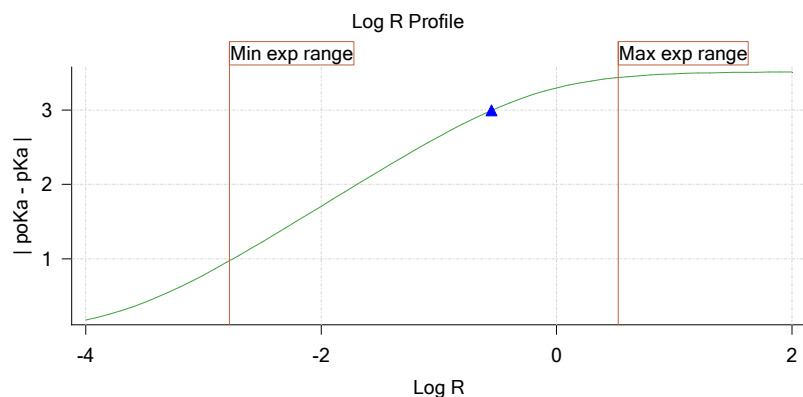
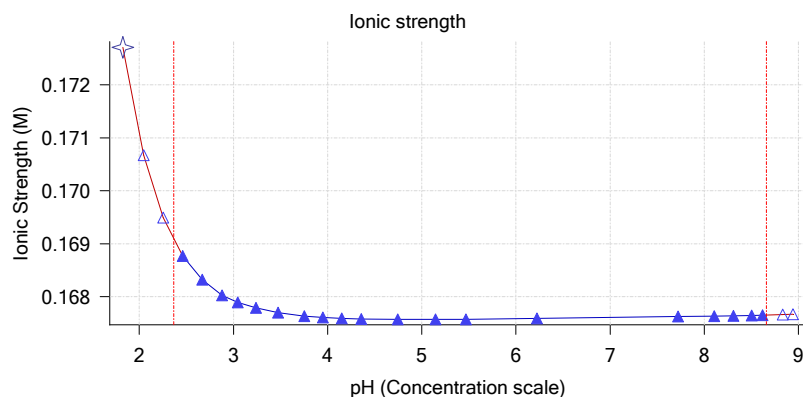
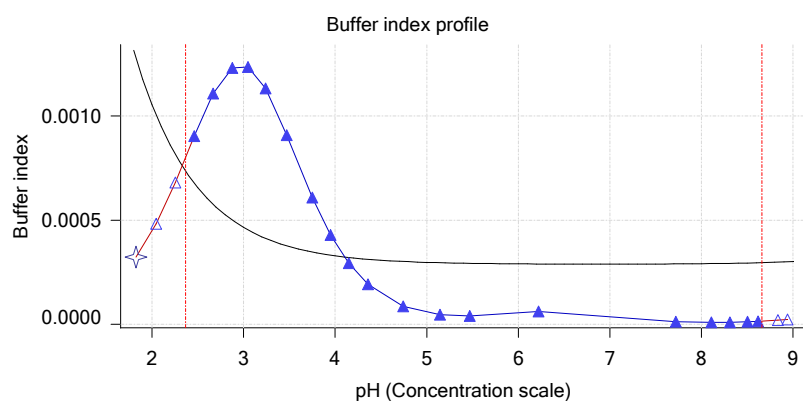
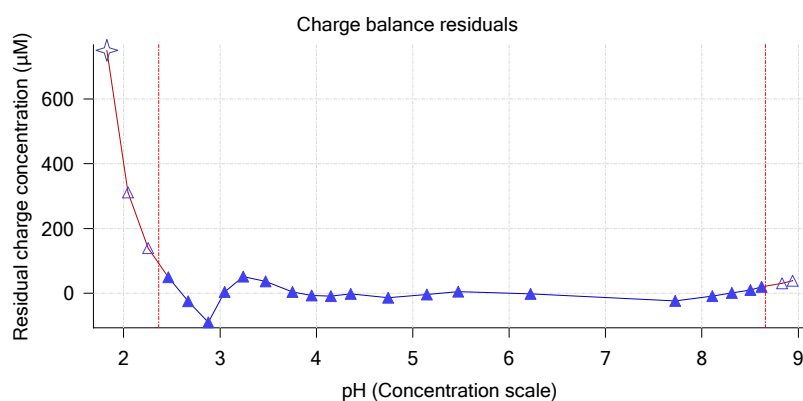
Other graphs



Sample name: **M04_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-24002**
 Filename: **C:\Sirius_T3\Mehtap\20180323_exp33_logP_T3-2\18C-24002_M04_octanol_pH-metric high logP.t3r**

Experiment start time: **3/24/2018 1:34:06 AM**
 Analyst: **Dorothy Levorse**
 Instrument ID: **T312060**

Other graphs (continued)



Sample name: **M04_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-24002**
 Filename: **C:\Sirius_T3\Mehtap\20180323_exp33_logP_T3-2\18C-24002_M04_octanol_pH-metric high logP.t3r**

Experiment start time: **3/24/2018 1:34:06 AM**
 Analyst: **Dorothy Levorse**
 Instrument ID: **T312060**

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	M04_octanol	3/9/2018 4:34:21 PM	User entered value
Sample by	Weight		Default value
Sample weight	0.001110 g	3/23/2018 5:00:32 PM	User entered value
Formula weight	269.73 g/mol	3/9/2018 4:34:21 PM	User entered value
Solubility	Unknown		Default value
Molecular weight	269.73	3/9/2018 4:34:21 PM	User entered value
Individual pKa ionic environments	No		Default value
Number of pKas	1	3/9/2018 4:34:21 PM	User entered value
Sample is a	Base	3/9/2018 4:34:21 PM	User entered value
pKa 1	5.97	3/9/2018 4:34:21 PM	User entered value
logp (XH +)	0.19	3/9/2018 4:34:33 PM	User entered value
logP (neutral X)	3.50	3/23/2018 2:32:46 PM	User entered value

Events

Time	Event	Water	Acid	Base	Octanol	pH	dpH/dt	pH R-squared	pH SD	dpH/dt time
5:00.2	Initial pH = 9.63									
7:59.7	Data point 1	1.50000 mL	0.04892 mL	0.00183 mL	0.03001 mL	2.014	-0.00160	0.32049	0.00014	10.5 s
8:46.4	Data point 2	1.50000 mL	0.04892 mL	0.01635 mL	0.03001 mL	2.224	-0.00074	0.14269	0.00010	10.0 s
9:21.9	Data point 3	1.50000 mL	0.04892 mL	0.02545 mL	0.03001 mL	2.429	0.00290	0.05785	0.00060	10.0 s
9:57.5	Data point 4	1.50000 mL	0.04892 mL	0.03109 mL	0.03001 mL	2.620	-0.00606	0.72611	0.00035	10.0 s
10:33.1	Data point 5	1.50000 mL	0.04892 mL	0.03478 mL	0.03001 mL	2.822	-0.00318	0.34754	0.00027	10.0 s
11:08.6	Data point 6	1.50000 mL	0.04892 mL	0.03718 mL	0.03001 mL	3.022	-0.00788	0.20158	0.00087	10.0 s
11:44.0	Data point 7	1.50000 mL	0.04892 mL	0.03883 mL	0.03001 mL	3.182	-0.00246	0.53024	0.00017	10.0 s
12:34.9	Data point 8	1.50000 mL	0.04892 mL	0.04052 mL	0.03001 mL	3.368	-0.01119	0.56806	0.00073	10.0 s
13:25.9	Data point 9	1.50000 mL	0.04892 mL	0.04182 mL	0.03001 mL	3.557	-0.00577	0.09662	0.00092	10.0 s
14:11.6	Data point 10	1.50000 mL	0.04892 mL	0.04294 mL	0.03001 mL	3.749	-0.00944	0.26941	0.00090	10.0 s
14:47.0	Data point 11	1.50000 mL	0.04892 mL	0.04393 mL	0.03001 mL	3.955	-0.00902	0.80462	0.00050	10.0 s
15:22.5	Data point 12	1.50000 mL	0.04892 mL	0.04497 mL	0.03001 mL	4.163	-0.00871	0.81314	0.00048	10.5 s
15:58.4	Data point 13	1.50000 mL	0.04892 mL	0.04600 mL	0.03001 mL	4.430	-0.01386	0.79748	0.00077	11.0 s
16:45.2	Data point 14	1.50000 mL	0.04892 mL	0.04673 mL	0.03001 mL	4.671	-0.00488	0.10408	0.00075	11.5 s
17:22.1	Data point 15	1.50000 mL	0.04892 mL	0.04711 mL	0.03001 mL	4.865	-0.01667	0.86899	0.00088	14.5 s
18:12.3	Data point 16	1.50000 mL	0.04892 mL	0.04751 mL	0.03001 mL	5.110	-0.01586	0.79314	0.00088	16.0 s
18:53.6	Data point 17	1.50000 mL	0.04892 mL	0.04770 mL	0.03001 mL	5.348	-0.01986	0.98346	0.00099	20.5 s
19:44.8	Data point 18	1.50000 mL	0.04892 mL	0.04795 mL	0.03001 mL	5.739	-0.01915	0.96564	0.00096	26.5 s
20:36.6	Data point 19	1.50000 mL	0.04892 mL	0.04807 mL	0.03001 mL	5.946	-0.01903	0.92495	0.00098	30.5 s
21:37.5	Data point 20	1.50000 mL	0.04892 mL	0.04819 mL	0.03001 mL	6.643	-0.02497	0.94842	0.00127	Timed out at 59.5 s
23:08.1	Data point 21	1.50000 mL	0.04892 mL	0.04833 mL	0.03001 mL	8.221	-0.07094	0.99161	0.00352	Timed out at 59.5 s
24:43.7	Data point 22	1.50000 mL	0.04892 mL	0.04840 mL	0.03001 mL	8.555	-0.03178	0.97425	0.00159	Timed out at 59.5 s
26:19.4	Data point 23	1.50000 mL	0.04892 mL	0.04847 mL	0.03001 mL	8.794	-0.01850	0.95661	0.00093	58.5 s
27:48.5	Data point 24	1.50000 mL	0.04892 mL	0.04857 mL	0.03001 mL	9.039	-0.01975	0.95215	0.00100	41.5 s
29:30.0	Data point 25	1.50000 mL	0.10310 mL	0.04857 mL	0.11002 mL	1.964	-0.00880	0.24648	0.00088	10.0 s
30:16.3	Data point 26	1.50000 mL	0.10310 mL	0.06510 mL	0.11002 mL	2.166	-0.01564	0.64906	0.00096	11.0 s
30:53.0	Data point 27	1.50000 mL	0.10310 mL	0.07627 mL	0.11002 mL	2.359	-0.00237	0.24657	0.00024	10.5 s
31:29.0	Data point 28	1.50000 mL	0.10310 mL	0.08347 mL	0.11002 mL	2.587	0.00566	0.08086	0.00098	10.5 s
32:05.1	Data point 29	1.50000 mL	0.10310 mL	0.08784 mL	0.11002 mL	2.757	-0.00202	0.33078	0.00017	10.5 s
32:51.5	Data point 30	1.50000 mL	0.10310 mL	0.09118 mL	0.11002 mL	2.950	-0.00478	0.66757	0.00029	10.0 s
33:26.8	Data point 31	1.50000 mL	0.10310 mL	0.09346 mL	0.11002 mL	3.123	-0.00470	0.90243	0.00024	10.0 s
34:17.8	Data point 32	1.50000 mL	0.10310 mL	0.09579 mL	0.11002 mL	3.317	-0.00344	0.59909	0.00022	10.5 s
35:09.2	Data point 33	1.50000 mL	0.10310 mL	0.09755 mL	0.11002 mL	3.515	-0.00933	0.53854	0.00063	10.0 s
35:44.5	Data point 34	1.50000 mL	0.10310 mL	0.09894 mL	0.11002 mL	3.772	-0.00653	0.77129	0.00037	10.0 s
36:30.2	Data point 35	1.50000 mL	0.10310 mL	0.09979 mL	0.11002 mL	3.961	-0.00468	0.84923	0.00025	10.5 s
37:06.1	Data point 36	1.50000 mL	0.10310 mL	0.10031 mL	0.11002 mL	4.178	-0.00915	0.61492	0.00058	10.0 s
37:41.5	Data point 37	1.50000 mL	0.10310 mL	0.10071 mL	0.11002 mL	4.385	-0.00988	0.57323	0.00064	10.0 s



Assay Events

Sample name: **M04_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-24002**
Filename: **C:\Sirius_T3\Mehtap\20180323_exp33_logP_T3-2\18C-24002_M04_octanol_pH-metric high logP.t3r**

Experiment start time: **3/24/2018 1:34:06 AM**
Analyst: **Dorothy Levorse**
Instrument ID: **T312060**

Events (continued)

Time	Event	Water	Acid	Base	Octanol	pH	dpH/dt	pH R-squared	pH SD	dpH/dt time
38:16.9	Data point 38	1.50000 mL	0.10310 mL	0.10101 mL	0.11002 mL	4.612	-0.00861	0.68608	0.00051	10.5 s
38:52.8	Data point 39	1.50000 mL	0.10310 mL	0.10122 mL	0.11002 mL	4.835	-0.01226	0.66939	0.00074	10.5 s
39:28.7	Data point 40	1.50000 mL	0.10310 mL	0.10136 mL	0.11002 mL	5.051	-0.01367	0.71800	0.00080	11.0 s
40:05.1	Data point 41	1.50000 mL	0.10310 mL	0.10146 mL	0.11002 mL	5.292	-0.01155	0.59589	0.00074	12.0 s
40:47.6	Data point 42	1.50000 mL	0.10310 mL	0.10153 mL	0.11002 mL	5.555	-0.01710	0.84028	0.00092	13.5 s
41:31.6	Data point 43	1.50000 mL	0.10310 mL	0.10160 mL	0.11002 mL	5.972	-0.01840	0.92739	0.00094	31.0 s
42:33.2	Data point 44	1.50000 mL	0.10310 mL	0.10165 mL	0.11002 mL	6.512	-0.01880	0.91936	0.00097	53.0 s
43:51.7	Data point 45	1.50000 mL	0.10310 mL	0.10169 mL	0.11002 mL	7.037	-0.04193	0.98601	0.00209	Timed out at 59.5 s
45:22.1	Data point 46	1.50000 mL	0.10310 mL	0.10174 mL	0.11002 mL	7.209	-0.04636	0.98987	0.00230	Timed out at 59.5 s
46:52.7	Data point 47	1.50000 mL	0.10310 mL	0.10179 mL	0.11002 mL	7.847	-0.06759	0.99607	0.00335	Timed out at 59.5 s
48:23.2	Data point 48	1.50000 mL	0.10310 mL	0.10183 mL	0.11002 mL	8.503	-0.03401	0.99546	0.00168	Timed out at 59.5 s
49:53.7	Data point 49	1.50000 mL	0.10310 mL	0.10188 mL	0.11002 mL	8.608	-0.01529	0.60040	0.00097	47.5 s
51:11.7	Data point 50	1.50000 mL	0.10310 mL	0.10193 mL	0.11002 mL	8.772	-0.01850	0.93390	0.00095	52.0 s
52:34.3	Data point 51	1.50000 mL	0.10310 mL	0.10200 mL	0.11002 mL	9.026	-0.01279	0.96553	0.00064	36.5 s
54:34.0	Data point 52	1.50000 mL	0.16030 mL	0.10200 mL	0.51002 mL	1.954	-0.00445	0.52317	0.00030	10.0 s
55:20.3	Data point 53	1.50000 mL	0.16030 mL	0.12112 mL	0.51002 mL	2.166	0.01490	0.84480	0.00080	10.0 s
55:56.0	Data point 54	1.50000 mL	0.16030 mL	0.13304 mL	0.51002 mL	2.372	0.00293	0.49233	0.00021	10.5 s
56:32.0	Data point 55	1.50000 mL	0.16030 mL	0.14080 mL	0.51002 mL	2.578	0.01404	0.59238	0.00090	10.0 s
57:07.6	Data point 56	1.50000 mL	0.16030 mL	0.14593 mL	0.51002 mL	2.782	-0.00325	0.08785	0.00054	10.0 s
57:43.1	Data point 57	1.50000 mL	0.16030 mL	0.14953 mL	0.51002 mL	2.990	-0.00261	0.10471	0.00040	10.0 s
58:18.5	Data point 58	1.50000 mL	0.16030 mL	0.15216 mL	0.51002 mL	3.158	-0.00222	0.09026	0.00037	10.0 s
59:04.3	Data point 59	1.50000 mL	0.16030 mL	0.15433 mL	0.51002 mL	3.351	-0.00880	0.28962	0.00081	10.0 s
59:39.8	Data point 60	1.50000 mL	0.16030 mL	0.15600 mL	0.51002 mL	3.582	-0.01386	0.91128	0.00072	10.5 s
1:00:15.8	Data point 61	1.50000 mL	0.16030 mL	0.15722 mL	0.51002 mL	3.861	-0.01252	0.59534	0.00080	10.0 s
1:00:56.3	Data point 62	1.50000 mL	0.16030 mL	0.15779 mL	0.51002 mL	4.058	-0.00480	0.17045	0.00057	10.0 s
1:01:42.1	Data point 63	1.50000 mL	0.16030 mL	0.15818 mL	0.51002 mL	4.256	-0.00431	0.26492	0.00041	10.0 s
1:02:32.9	Data point 64	1.50000 mL	0.16030 mL	0.15849 mL	0.51002 mL	4.464	0.00183	0.00838	0.00099	18.5 s
1:03:16.7	Data point 65	1.50000 mL	0.16030 mL	0.15873 mL	0.51002 mL	4.850	-0.01054	0.48317	0.00075	10.5 s
1:03:57.8	Data point 66	1.50000 mL	0.16030 mL	0.15889 mL	0.51002 mL	5.251	-0.01079	0.55670	0.00071	12.0 s
1:04:40.3	Data point 67	1.50000 mL	0.16030 mL	0.15898 mL	0.51002 mL	5.574	-0.01750	0.78457	0.00098	15.0 s
1:05:25.7	Data point 68	1.50000 mL	0.16030 mL	0.15910 mL	0.51002 mL	6.324	-0.01848	0.97545	0.00092	54.0 s
1:06:50.3	Data point 69	1.50000 mL	0.16030 mL	0.15924 mL	0.51002 mL	7.819	-0.10642	0.99284	0.00528	Timed out at 59.5 s
1:08:25.9	Data point 70	1.50000 mL	0.16030 mL	0.15931 mL	0.51002 mL	8.203	-0.07202	0.98050	0.00359	Timed out at 59.5 s
1:09:56.4	Data point 71	1.50000 mL	0.16030 mL	0.15936 mL	0.51002 mL	8.406	-0.04547	0.97923	0.00227	Timed out at 59.5 s
1:11:26.8	Data point 72	1.50000 mL	0.16030 mL	0.15941 mL	0.51002 mL	8.600	-0.01814	0.81212	0.00099	42.0 s
1:12:39.4	Data point 73	1.50000 mL	0.16030 mL	0.15945 mL	0.51002 mL	8.714	-0.02169	0.85709	0.00116	Timed out at 59.5 s
1:14:15.1	Data point 74	1.50000 mL	0.16030 mL	0.15953 mL	0.51002 mL	8.928	-0.01718	0.73352	0.00099	26.0 s
1:15:11.8	Data point 75	1.50000 mL	0.16030 mL	0.15957 mL	0.51002 mL	9.035	-0.01441	0.58124	0.00093	19.5 s
1:15:40.3	Assay volumes	1.50000 mL	0.16030 mL	0.15957 mL	0.51002 mL					

Sample name: **M04_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-24002**
 Filename: **C:\Sirius_T3\Mehtap\20180323_exp33_logP_T3-2\18C-24002_M04_octanol_pH-metric high logP.t3r**

Experiment start time: **3/24/2018 1:34:06 AM**
 Analyst: **Dorothy Levorse**
 Instrument ID: **T312060**

Assay Settings

Setting	Value	Original Value	Date/Time changed	Imported from
General Settings				
Analyst name	Dorothy Levorse			
Standard Experiment Settings				
Number of titrations	3			
Minimum pH	2.000			
Maximum pH	9.000			
pH step between points of	0.200			
Minimum titrant addition	0.00002 mL			
Maximum titrant addition	0.10000 mL			
Argon flow rate	100%			
Start titration using	Cautious pH adjust			
Advanced General Settings				
Detect turbidity using	None			
Collect turbidity sensor data	No			
Collect UV spectra	No			
Stir after titrant addition for	5 seconds			
For titrant addition, stir at	10%			
Titrant Pre-Dose				
Titrant pre-dose	None			
Assay Medium				
ISA water volume	1.50 mL			
Water added	Automatic			
Partition solvent type	Octanol			
Partition volume	0.030 mL			
Partition solvent added	Automatic			
After partition addition, stir for	1 seconds			
Sample Sonication				
Sonicate	Yes			
Adjust pH for sonication	No			
Sonicate for	60 seconds			
After sonication stir for	5 seconds			
Sample Dissolution				
Perform a dissolution stage	Yes			
Adjust and hold pH for dissolution	To start pH			
Stir to dissolve for	120 seconds			
For dissolution, stir at	10%			
Carbonate purge				
Perform a carbonate purge	No			
Temperature Control				
Wait for temperature	Yes			
Required start temperature	25.0°C			
Acceptable deviation	0.5°C			
Time to wait	60 seconds			
Stir speed of	50%			
Titration 1				
Titrate from	Low to high pH			
Adjust to start pH	Yes			
After pH adjust stir for	30 seconds			
Stir to allow partitioning for	15 seconds			
Stirrer speed for partitioning	50%			
Titration 2				
Titrate from	Low to high pH			
Add additional water	0.00 mL			
Additional partition solvent volume	0.080 mL			
Additional partition solvent added	Automatic			
After pH adjust stir for	30 seconds			
Stir to allow partitioning for	15 seconds			
Stirrer speed for partitioning	55%			

Sample name: **M04_octanol**
 Assay name: **pH-metric high logP**
 Assay ID: **18C-24002**
 Filename: **C:\Sirius_T3\Mehtap\20180323_exp33_logP_T3-2\18C-24002_M04_octanol_pH-metric high logP.t3r**

Experiment start time: **3/24/2018 1:34:06 AM**
 Analyst: **Dorothy Levorse**
 Instrument ID: **T312060**

Assay Settings (continued)

Setting	Value	Original Value	Date/Time changed	Imported from
Titration 3				
Titrate from	Low to high pH			
Add additional water	0.00 mL			
Additional partition solvent volume	0.400 mL			
Additional partition solvent added	Automatic			
After pH adjust stir for	30 seconds			
Stir to allow partitioning for	15 seconds			
Stirrer speed for partitioning	60%			
Data Point Stability				
Stir during data point collection	No			
Delay before data point collection	0 seconds			
Number of points to average	20 points			
Time interval between points	0.50 seconds			
Required maximum standard deviation	0.00100 dpH/dt			
Stability timeout after	60 seconds			

Calibration Settings

Setting	Value	Date/Time changed	Imported from
Four-Plus alpha	0.119	3/24/2018 1:34:06 AM	C:\Sirius_T3\HCl18C23.t3r
Four-Plus S	0.9972	3/24/2018 1:34:06 AM	C:\Sirius_T3\HCl18C23.t3r
Four-Plus jH	0.9	3/24/2018 1:34:06 AM	C:\Sirius_T3\HCl18C23.t3r
Four-Plus jOH	-0.3	3/24/2018 1:34:06 AM	C:\Sirius_T3\HCl18C23.t3r
Base concentration factor	1.003	3/24/2018 1:34:06 AM	C:\Sirius_T3\KOH18C23.t3r
Acid concentration factor	0.997	3/24/2018 1:34:06 AM	C:\Sirius_T3\HCl18C23.t3r

Instrument Settings

Setting	Value	Batch Id	Install date
Instrument owner	Merck		
Instrument ID	T312060		
Instrument type	T3 Simulator		
Software version	1.1.3.0		
Dispenser module		T3DM1200361	3/31/2009 6:24:52 AM
Dispenser 0	Water		3/31/2009 6:25:05 AM
Syringe volume	2.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Water (0.15 M KCl)	02-06-2018	3/16/2018 11:09:18 AM
Dispenser 2	Acid		3/31/2009 6:25:11 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Acid (0.5 M HCl)	03-16-2018	3/16/2018 10:56:23 AM
Dispenser 1	Base		3/31/2009 6:25:21 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Base (0.5 M KOH)	3/22/2018	3/23/2018 9:34:17 AM
Dispenser 5	Cosolvent		3/31/2009 6:26:24 AM
Syringe volume	2.5 mL		
Firmware version	1.2.1(r2)		
Distribution valve 5	Distribution Valve		3/31/2009 6:28:19 AM
Firmware version	1.1.3		
Port A	Methanol (80%, 0.15 M KCl)	02-08-2018	3/6/2018 10:28:59 AM
Port B	Cyclohexane	11-01-17	2/27/2018 11:37:57 AM
Dispenser 3	Buffer		8/3/2010 6:05:16 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Dodecane	2018/01/31	2/28/2018 11:18:04 AM
Dispenser 6	Octanol		10/22/2010 11:52:43 AM

Sample name: **M04_octanol** Experiment start time: **3/24/2018 1:34:06 AM**
 Assay name: **pH-metric high logP** Analyst: **Dorothy Levorse**
 Assay ID: **18C-24002** Instrument ID: **T312060**
 Filename: **C:\Sirius_T3\Mehtap\20180323_exp33_logP_T3-2\18C-24002_M04_octanol_pH-metric high logP.t3r**

Instrument Settings (continued)

Setting	Value	Batch Id	Install date
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Octanol	01-31-2018	2/27/2018 10:59:35 AM
Titrator		T3TM1200161	3/31/2009 6:24:17 AM
Horizontal axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Vertical axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Chassis I/O firmware version	1.11 AI1DI0DO4 Norgren I/O		
Probe I/O firmware version	1.1.1		
Electrode	T3 Electrode	T3E0923	1/23/2018 3:01:00 PM
E0 calibration	+4.89 mV		3/24/2018 1:34:34 AM
Filling solution	3M KCl	KCL097	3/23/2018 9:29:07 AM
Liquids			
Wash 1	50% IPA:50% Water		3/23/2018 9:29:12 AM
Wash 2	0.5% Triton X-100 in H2O		3/23/2018 9:29:15 AM
Buffer position 1	pH7 Wash		3/23/2018 9:29:19 AM
Buffer position 2	pH 7		3/23/2018 9:29:21 AM
Storage position			3/23/2018 9:30:23 AM
Wash water	7.7e+003 mL	03-12-2018	3/12/2018 9:25:04 AM
Waste	2.5e+003 mL		3/12/2018 9:24:49 AM
Temperature controller			8/5/2010 7:35:13 AM
Turbidity detector			3/31/2009 6:24:45 AM
Spectrometer		074811	11/23/2010 12:22:28 PM
Dip probe		10196	
Wavelength coefficient A0	183.333		
Wavelength coefficient A1	2.21568		
Wavelength coefficient A2	-0.000289308		
Total lamp lit time	162:53:01		11/23/2010 12:22:28 PM
Calibrated on	2/27/2018 11:40:38 AM		
Integration time	40		
Scans averaged	10		
Autoloader		T3AL1200345	11/10/2015 10:34:13 AM
Left-right axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Front-back axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Vertical axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Chassis I/O firmware version	1.11 AI1DI0DO4 Norgren I/O		
Configuration			
Alternate titration position	Titration position		
Alternate reference position	Reference position		
Maximum standard vial volume	3.50 mL		
Maximum alternate vial volume	25.00 mL		
Automatic action idle period	5 minute(s)		
Titrant tube volume	1.3 mL		
Syringe flush count	3.50		
Flowing wash pump volume	20.0 mL		
Flowing wash stir duration	5 s		
Flowing wash stir speed	30%		
Solvent wash stir duration	5 s		
Solvent wash stir speed	30%		
Surfactant wash stir duration	5 s		
Surfactant wash stir speed	30%		
E0 calibration minimum number of points	10		
E0 calibration maximum standard deviation	0.01500		
E0 calibration timeout period	60 s		
E0 calibration stir duration	5 s		
E0 calibration preparation stir speed	30%		
E0 calibration buffer wash stir duration	5 s		
E0 calibration buffer wash stir speed	30%		
E0 calibration reading stir speed	0%		



Assay Settings

Sample name: **M04_octanol** Experiment start time: **3/24/2018 1:34:06 AM**
Assay name: **pH-metric high logP** Analyst: **Dorothy Levorse**
Assay ID: **18C-24002** Instrument ID: **T312060**
Filename: **C:\Sirius_T3\Mehtap\20180323_exp33_logP_T3-2\18C-24002_M04_octanol_pH-metric high logP.t3r**

Instrument Settings (continued)

Setting	Value	Batch Id	Install date
Spectrometer calibration stir duration	5 s		
Spectrometer calibration stir speed	30%		
Spectrometer calibration wash pump volume	20.0 mL		
Spectrometer calibration wash stir duration	5 s		
Spectrometer calibration wash stir speed	30%		
Overhead dispense height	10000		

Refinement Settings

Setting	Value	Default value
Turbidity detection method	None	None
Turbidity wavelength to assess	500.0 nm	500.0 nm
Turbidity maximum absorbance	0.100	0.100
Turbidity probe threshold	50.00	50.00